HW 3
CHEM 362

Due: Oct 9, 2019

1. The theoretical lattice energy equation is shown.

$$U = \frac{NM_{NaCl}Z^2e^2}{4\pi\varepsilon_o r_o}\left(1-\frac{1}{n}\right)$$

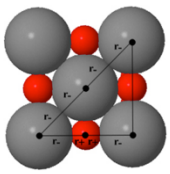
   a. Which factors are dependent on the identities of the atoms that make up the solid?
   b. What is a Madelung constant? Why can the same Madelung constant be used for seemingly different substances?

2. Use Figure 4-2 in Cotton as a guide and write out balanced chemical equations for each step in the Born-Haber cycle of MgO. Using the given data, determine the lattice energy.

   For Mg (s), **Δ** Hsub = +148 kJ/mol
   Bond dissociation energy for O_2 = +499 kJ/mol
   1st ionization energy for Mg = +738 kJ/mol;
   2nd ionization energy for Mg = +1450 kJ/mol;
   1st electron affinity enthalpy for O = –141 kJ/mol;
   2nd electron affinity enthalpy for O = +748 kJ/mol
   For MgO (s), enthalpy of formation = –602 kJ/mol

3. Study the unit cell drawings found in Cotton chapter 4 for NaCl, zinc blende, rutile, CsCl and fluorite. Now by the location of each atom type in the unit cell (corner, edge, face or internal) add up all the contributions from these atoms to show how the empirical formula is arrived at.
   Hint: corner atoms are shared by eight unit cells, edges are shared by four unit cells, face atoms are shared by two unit cells and internal atoms belong to only one unit cell.

4. Derive the radius ratio ideal value for NaCl type structures (CN=6)
   Hint: see the figure to the right.



5. Using the radius ratio approach, predict coordination numbers for LiF, LiCl, LiBr, NaBr and KBr. Explain using words and figures (*Hint: consider geometry, size of ions and stability)* why these differences in coordination numbers exist.

6. Using drawings, show the difference between cubic and hexagonal close packing.

7. What are the three types of cubic unit cells? Sketch them, and describe the similarities/differences